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Conservative Supra-Characteristics Method
For Splitting the Hyperbolic Systems of
Gasdynamics for Real and Perfect Gases

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C.K. Lombard

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For Splitting the Hyperbolic Systems of
Gasdynamics for Real and Perfect Gases

C.K. Lombard
PEDA Corporation
1150 Fife Street
Palo Alto, CA 94301

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National Aeronautics and
Space Administration

Ames Research Center
Moffett Field, California 94035

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Abstract

A new conservative flux difference splitting is presented for the hyperbolic systems of gasdynamics. The stable robust method is suitable for wide application in a variety of schemes, explicit or implicit, iterative or direct, for marching in either time or space. The splitting is modeled on the local quasi one dimensional characteristics system for multi-dimensional flow similar to Chakravarthy's nonconservative split coefficient matrix method (SCM); but, as the result of maintaining global conservation, the method is able to capture sharp shocks correctly. The embedded characteristics formulation is cast in a primitive variable the volumetric internal energy (rather than the pressure) that is effective for treating real as well as perfect gases. Finally the relationship of the splitting to characteristics boundary conditions is discussed and the associated conservative matrix formulation for a computed blown wall boundary condition is developed as an example.

The theoretical development employs and extends the notion of Roe of constructing stable upwind difference formulae by "sending" split simple one sided flux difference pieces to appropriate mesh sites. The developments are also believed to have the potential for aiding in the analysis of both existing and new conservative difference schemes.

Acknowledgements

The author wishes to acknowledge many stimulating discussions of Roe's method and upwind difference schemes with Professor Joseph Oliger of Stanford University who served as a consultant. Equally helpful has been the enthusiastic collaboration of Jaw Yen Yang in checking derivations and in programming and testing the method in model problems. During the course of this research, to which he is making additional contributions for his dissertation, Yang has been a Stanford Ph.D. candidate under Professor Daniel Bershader. Many earlier discussions of the effectiveness of characteristic boundary conditions and Lax-Wendroff type hybrid characteristic-conservative methods with Thomas Coakley of NASA-Ames Research Center were a strong motivating influence behind the work reported here.

RESEARCH REPORT

CONSERVATIVE SUPRA-CHARACTERISTICS METHOD FOR SPLITTING THE HYPERBOLIC SYSTEMS OF GASDYNAMICS FOR REAL AND PERFECT GASES

by

C.K. Lombard

I. Introduction

For many years, Morretti^{1,2,3} (see also Pandolfi and Zanetti⁴) has advocated and demonstrated the physical content and accuracy available in the nonconservative primitive equations of gasdynamics and particularly the characteristics formulation of those equations, especially at boundaries. Following closely upon the Morretti " λ scheme" Chakravarthy^{5,6}, et al came forth with a simplified multidimensional, quasi one dimensional method based on eigenvector splittings of the coefficient matrices of the nonconservative Euler equations. Chakravarthy emphasized the correspondence between stable upwind differencings of the split equation pieces and the transformed quasi one dimensional characteristic relations. Getting generally very attractive results including very sharp captured shock transitions, Chakravarthy encountered only one substantial problem, that of unreliable shock location.

On the other hand, a theorem of Lax and Wendroff⁷ that a finite difference scheme in conservation law form can realize the Rankine-Hugoniot jump conditions automatically has led to a long line of development featuring such popular schemes as those of MacCormack^{8,9}, Beam and Warming¹⁰,

and Briley and McDonald¹¹. However, such conservative shock capturing schemes have been found deficient in resolution, tending to smear the transitions over several mesh points, and are subject to stability plaguing overshoots and undershoots and nonphysical solutions all of which must be controlled by the addition of ad hoc artificial dissipation terms. Finally the artificial dissipation coupled with indiscriminant directional differencing has led to excessive smearing of contact discontinuities.

Recent recognition of these drawbacks has led to the introduction of directional signal propagation information in conservative schemes. The principal lines of development appear to be flux splitting introduced first by Steger and Warming^{12,13} and more recently flux difference splitting, put forth by Enquist and Osher¹⁴, Osher and Solomon¹⁵, and by Roe¹⁶. Most recently Reklis and Thomas¹⁷ have presented an upwind control volume centered method that appears to be a hybrid of flux splitting and flux difference splitting. With the exception of the latter, these methods have been surveyed and appraised by van Leer¹⁸ and by Harten, Lax and van Leer¹⁹. Flux splitting suffers from the flaw that it fails to provide consistent directional signal information where it is most needed, namely in the vicinity of a change in eigenvalue sign. Flux difference splitting on the other hand admits a greater generality than flux splitting and can be tailored to a variety of signal propagating philosophies or requirements as partially expressed in the works to date and the present report.

The approach taken in the present work is to unify in so far as possible the virtues of the signal propagation of the characteristics method with simple conservative upwind finite difference schemes in a way that

permits both explicit and implicit numerical methods. Among motivations for choosing the characteristics based splitting presented here is the belief that it is the natural and most numerically robust linearization of the gasdynamic equations since it supports the physical directional propagation of sound waves. This belief also seems to be supported by various gedanken experiments performed on numerical flow simulation pathologies conceived out of past experience with conservative methods.

In the characteristics interpretation and approach, the present method is closest to Chakravarthy; and in the development of general conservative upwind schemes out of one sided differences, follows Roe. Explicitly, reliance is placed on Roe's property U which the new matrix shares with his, though they are very different both in detail and concept of construction. The principal feature of property U for admitting Rankine-Hugoniot satisfying shock transitions is

$$\Delta F \equiv \tilde{A} \Delta q \quad (1)$$

where ΔF expresses the flux difference on either side of the transition and Δq is the corresponding jump in the conservative variable vector. We find it more than mildly interesting that conservative methods based on this matrix, namely,

$$\delta q + \tilde{A} \Delta q = 0 \quad (2)$$

are in the same form for method of solution as in their linear stability analysis.

II. Conservative Supra-Characteristics Method

Our method for constructing \tilde{A} rests on the observation that differences of nonlinear quantities such as ρu appearing in the conservative equations can be expressed exactly as

$$\Delta \rho u = \bar{\rho} \Delta u + \bar{u} \Delta \rho . \quad (3)$$

This fact was recognized by Roe but the tougher triad terms evidently caused him to take a different ad hoc approach which he noted was generalizable to other hyperbolic systems. The key to sorting out how to construct a splittable \tilde{A} from simple end point averagings ($\bar{}$) of quantities across an interval is to analyze in detail how the characteristic equations are formed of the nonconservative primitive equations, on the one hand, and how the conservative equations are formed out of the primitive ones, on the other. The results will be sketched below but the cumbersome details are left to the Appendix. Here, we only remark that \tilde{A} is definitely not \bar{A} , which van Leer has tried and regards as too dissipative¹⁹.

Conservation And The Elemental Interval Equation

Before describing the present \tilde{A} further, we introduce some relevant background material. The first item is the general discrete quasi one dimensional simple interval difference equation as an element of a multi-dimensional globally conservative numerical procedure. This concept is regarded as central to Roe's approach but is not introduced by him in this way. In the text figure below we see a bounded one dimensional computational domain divided up by interior mesh points into N-1 simple

intervals. We place data on the computed boundaries which are treated naturally with characteristic boundary conditions by this method, as will be described in a later section.

$$\begin{array}{ccccccc} \{ & (1) & \cdot & (2) & \cdot & , , , & \cdot & (N-1) & \} \\ 1 & & 2 & & 3 & & & N-1 & N \end{array}$$

The simple (j)th interval equation whose splittings form the building blocks of the nodal point difference equations is then

$$(J \delta_{\tau}^* q)_j + (\Delta_{\xi} F)_j = 0 \quad (4)$$

Here J is the volume of a slab from a computational topological cube bounded by all the adjacent mesh points to one at the center and isolated by passing a ξ constant coordinate surface through the center point. In one dimension J is just Δx_j . In multidimensions the "cube" (area in 2-D) is bisected into slabs for each of the general curvilinear coordinate directions. For each slab and coordinate direction there exist elemental equations of the form (4). In the equation the term $\delta_{\tau}^* q_j$ is a measure of the change in the conservative variable q vector over the interval $\Delta \xi$ in the slab as a result of the bounding inviscid flux difference $\Delta_{\xi} F$. (Note the discrete computational flux F_{ξ} contains the associated slab face area S_{ξ} . For a discussion of 2-D and 3-D discrete finite volume formulations of the conservative equations in generalized curvilinear coordinates on a finite difference mesh see Lombard, Davy, and Green²⁰ and Thomas and Lombard²¹.) When such equations (4) are summed over all mesh intervals in all coordinate directions,

all the interior flux terms cancel identically , and there results the discrete approximation to the global conservation law for the computational domain

$$\int_V \dot{q} \, dV \approx \sum J \, \delta_\tau^* \dot{q} = - \sum \underline{F}_\sigma \cdot \underline{n} \approx - \iint_\sigma \underline{F} \cdot \underline{n} \, dS \quad . \quad (5)$$

Thus, when difference equations are constructed among split pieces of the elemental difference equations (4), global conservation requires only that the weighting functions for the distribution of each piece among the nodal difference equations should sum to one for each elemental equation.

While Roe focused his attention exclusively on just the flux term of equation (4), it is true that all discrete quasi-one-dimensional conservative numerical methods can be constructed from the elemental difference equations (4). Within this context, the difference between methods resides not just in the treatment of the flux term $\nabla_\xi F$ but also in the definition of the unsteady term $\delta_\tau^* \dot{q}$. For example for all methods constructed of simple one sided differences, \dot{q}^* can be represented as

$$(\dot{q}^*)_j = \alpha q_j + (1 - \alpha) q_{j+1} \quad . \quad (6)$$

In MacCormack's method, for instance, $\alpha = \frac{1}{2}$. We will see presently that the way methods treat characteristic information is, or ought to be, reflected in the weighting function α .

Stable Scalar Convection Equations

The second item is the scalar convection equation which is well known to admit stable explicit and implicit numerical schemes when

backward or forward differenced according as the sign of the eigenvalue is positive or negative as below

$$\delta_{\tau} u_j + \lambda \nabla_{\xi} u_j = 0, \quad \lambda \geq 0 \quad (7)$$

$$\delta_{\tau} u_j + \lambda \Delta_{\xi} u_j = 0, \quad \lambda \leq 0$$

Supra-Characteristics Matrix Splitting

To continue with the discussion of the matrix that linearizes the flux difference equation (1), we are able to express \tilde{A} as

$$\tilde{A} = M T D T^{-1} \tilde{M}^{-1} \quad (8)$$

Here the matrices M , T and T^{-1} bear considerable formal correspondence to the matrices of flux splitting^{12,13} but \tilde{M}^{-1} is very different from the inverse M^{-1} . Specifically, \tilde{M}^{-1} is the matrix operator that constructs the right hand side (spatial) difference vector of the nonconservative primitive equations from the associated conservative variable vector differences. The matrix T^{-1} is the operator that transforms the primitive equations into the scalar characteristic equations. Indeed, with reference to equation (4), we can write the 1-D elemental characteristics equations that underlie the present conservative method as the set

$$J D T^{-1} M^{-1} \delta_{\tau}^* q + D T^{-1} \tilde{M}^{-1} \Delta_{\xi} q = 0 \quad (9)$$

In these equations, the diagonal matrix D is not the eigenvalue

matrix but a truth function which for a complete set of eigenvalues is the identity matrix. This formulation permits treating all the difference terms of the primitive equations exactly without source terms and has led us to conceive the nomer conservative "supra(above, akin to)-characteristics" method (CSCM). To effect stable upwind difference methods the elemental characteristics equations are divided up for the j th interval according to partitioning the truth function D for positive and negative eigenvalues into D^+ and D^- with complementary ones and zeroes on the diagonals. In analogy with equations (7) the stable one sided first order splittings of equations (9) are

$$\begin{aligned} (J D^+ T^{-1} M^{-1})_j \delta_\tau q_{j+1} + (D^+ T^{-1} \tilde{M}^{-1} \Delta_\xi q)_j &= 0 \\ (J D^- T^{-1} M^{-1})_j \delta_\tau q_j + (D^- T^{-1} \tilde{M}^{-1} \Delta_\xi q)_j &= 0 \end{aligned} \quad (10)$$

Note for the elemental interval j the forward difference $\Delta_\xi q_j$ is equal to the backward difference $\nabla_\xi q_{j+1}$.

The stable conservative elemental difference equation pieces for the interval j are derived from equations (10) by multiplying by the matrix product $M T$. These, respectively from the right, serve to transform characteristics equations to primitive equations and primitive equations to conservative equations. The resulting splitting of equation (4) can be written

$$\begin{aligned} (J \tilde{A}^+)_j \delta_\tau q_{j+1} + (\tilde{A}^+ \Delta_\xi q)_j &= 0 \\ (J \tilde{A}^-)_j \delta_\tau q_j + (\tilde{A}^- \Delta_\xi q)_j &= 0 \end{aligned} \quad (11)$$

Comparing these with equations (4) makes it evident that for a characteristics based splitting the elemental interval measure of the conservative variable vector \tilde{q}_j^* for the unsteady term is defined (see (6)) as

$$\tilde{q}_j^* = \tilde{A}^- q_j + \tilde{A}^+ q_{j+1} . \quad (12)$$

With equations (11) as the basic stable elements and in analogy with Roe's prescription for "sending" the flux difference pieces $\tilde{A}^+ \Delta q$ and $\tilde{A}^- \Delta q$, a host of stable conservative upwind methods can be constructed.

In particular, a stable first order difference equation based on the elemental interval splitting (11) is

$$[(J \tilde{A}^+)_{j-1} + (J \tilde{A}^-)_j] \delta_\tau q_j + (\tilde{A}^+ \Delta_\xi q)_{j-1} + (\tilde{A}^- \Delta_\xi q)_j = 0 \quad (13)$$

Equation (13) is amenable to both explicit numerical methods involving a block diagonal matrix inversion and fully implicit methods involving block tridiagonal matrix inversions. Similarly a stable second order difference equation is

$$\begin{aligned} & \frac{1}{2} [-(J \tilde{A}^+)_{j-2} + 3(J \tilde{A}^+)_{j-1} + 3(J \tilde{A}^-)_j - (J \tilde{A}^-)_{j+1}] \delta_\tau q_j \\ & + \frac{1}{2} [-(\tilde{A}^+ \Delta_\xi q)_{j-2} + 3(\tilde{A}^+ \Delta_\xi q)_{j-1} + 3(\tilde{A}^- \Delta_\xi q)_j - (\tilde{A}^- \Delta_\xi q)_{j+1}] = 0 \end{aligned} \quad (14)$$

Equation (14) is also amenable to explicit numerical methods and to implicit methods involving either block pentadiagonal inversions or block tridiagonal inversions, if the implicit convective terms are treated first order as in equation (13). Appropriate explicit and implicit

numerical methods and their stability for eigenvector split schemes have been discussed in references 12 and 13.

For the elemental difference intervals adjacent to boundaries the distribution of the splittings (11) of the elemental interval equations to form stable interior nodal point difference equations such as (13) leaves pieces

$$\begin{aligned} (J \tilde{A}^-)_1 \delta_\tau q_1 + (\tilde{A}^- \Delta_\xi q)_1 &= 0 \\ (J \tilde{A}^+)_{N-1} \delta_\tau q_N + (\tilde{A}^+ \Delta_\xi q)_{N-1} &= 0 \end{aligned} \tag{15}$$

unused. These elemental equation pieces which embody the outrunning characteristics to the left and right boundaries respectively can be used as natural elements to construct dissipative boundary point difference schemes that satisfy, with our interior point schemes, sufficiency conditions for stability of the coupled discrete initial boundary value problem, Olliger²². It is physically satisfying that the inclusion of these residual elemental equation pieces (15) for boundary point difference approximations is also necessary to close the global conservation property of the set of elemental difference equations to the computational boundaries.

The use of various akin space-time extrapolations from the interior has been discussed and analyzed for stability with different interior point schemes by Olliger and Sundström²³ and Gustafson and Olliger²⁴. Yee²⁵, in a report with a recent extensive survey, sketched an approach based on flux splitting that is similar to the method we now present.

III. Natural Characteristic Boundary Conditions

The diagonal matrices for interior nodal point difference equations such as (13) and (14) have a complete set of independent eigenvectors corresponding to the complete set of stable characteristics equations potentially available from either the right or left of the solution point depending on eigenvalue sign. At a computational boundary nodal point, however, only the stable subset of characteristics differenced from the interior and with negative eigenvalues for a left boundary and positive eigenvalues for a right, are applicable. Then, if there are N dependent variables in the conservative variable vector and only M stable characteristic relations available from the interior, we must specify $N-M$ auxiliary boundary condition relations among the dependent variables. Such numerical auxiliary boundary conditions reflect in number and kind the natural boundary conditions for the PDE. To extend the approach of Kentzer²⁶ to a conservative matrix method such as we have here, auxiliary boundary relations are time differenced and included in the $N \times N$ block matrix of the diagonal to replace the unavailable exterior characteristic relations \tilde{A}^+ for a left boundary and \tilde{A}^- for a right boundary. Without the introduction of these auxiliary boundary condition relations the split matrices \tilde{A}^\pm are singular.

The method is illustrated for an isothermal wall boundary with prescribed blowing. Experience has shown it is most natural to introduce the auxiliary boundary conditions at the level at which the characteristic equations are formed namely at the T^{-1} matrix level. We specialize the construction to 2-D with a lower wall boundary which we assume is an η constant curvilinear coordinate line.

From the Appendix, the matrix T^{-1} for the full set of characteristic relations is

$$\begin{array}{cccc}
 -\frac{1}{\rho} & 0 & 0 & \frac{1}{\gamma P} \\
 0 & \frac{\hat{\eta}_y}{\rho c} & -\frac{\hat{\eta}_x}{\rho c} & 0 \\
 0 & \frac{\hat{\eta}_x}{\rho c} & \frac{\hat{\eta}_y}{\rho c} & \frac{1}{\gamma P} \\
 0 & -\frac{\hat{\eta}_x}{\rho c} & -\frac{\hat{\eta}_y}{\rho c} & \frac{1}{\gamma P}
 \end{array}
 .$$

In the formulation this matrix is to be multiplied by the primitive equation time difference (column) vector $(\delta\rho, \rho\delta u, \rho\delta v, \delta P)^+$. (Here for generality and applicability to real gas flows P is not the pressure p but the related $\frac{P}{\gamma-1}$.) The resulting characteristic variable differences are by row: (1) the entropy, (2) the tangential velocity, and (3) and (4) are the P^+ and P^- normal pressure velocity compatibility relations respectively. The eigenvalues associated with these characteristics are \hat{W}^η , \hat{W}^η , $\hat{W}^\eta + \hat{\eta}c$, $\hat{W}^\eta - \hat{\eta}c$. For subsonic blowing (inflow) only the latter of these is negative and is associated with a stable difference relation from the interior. Thus, the first three characteristic difference relations associated with the first three rows of T^{-1} need to be replaced by auxiliary boundary conditions. Such boundary conditions do not involve differences to the interior but only relations which serve to constrain the mutual variations of the dependent variables at the boundary.

For consistency and global conservation with the interior point procedure, the boundary point computational procedure having the properties just described can conveniently be represented as

$$J M T(D^- T^{-1} M^{-1} + D^+ T' M')_1 \delta q_1 + (M T D^- T^{-1} M^{-1} \Delta_\xi q)_1 = 0 \quad (16)$$

Here for simplicity, first order differencing of the P^- characteristic has been assumed from the wall. The auxiliary boundary conditions are, quite evidently, embodied in the matrix $D^+ T' M'$ where D^+ is the truth function complement to D^- , T' is the matrix in which the boundary conditions are formulated, and M' permits the formulation to be flexibly constructed among either the primitive variable differences, the conservative variable differences, or more commonly a combination of the two.

Not too surprisingly it has been found that appropriate (stable) auxiliary boundary conditions have T' matrix representations row by row quite similar to the matrix rows of T^{-1} they naturally replace. Indeed for good matrix conditioning in the coupled difference equation boundary condition procedure, it is highly desirable that the correspondence be as close as possible. Consequently, in the following we elucidate the properties of T' in terms of the rows of T^{-1} that are naturally replaced.

The first row of T^{-1} (multiplied by the primitive variable vector differences) can be seen to represent a logarithmic differential relation of a thermodynamic function the entropy. Indeed, a viable auxiliary boundary condition that can be applied is constant entropy ($\delta \ln(\frac{P}{\rho}) = 0$), i.e. no wall heating, in which case row one of T^{-1} could be used intact for T' . A more general thermodynamic relation at the wall is the polytrope law $P \sim \rho^\alpha$ which can be logarithmically differenced with the matrix coefficients

$$-\frac{1}{\rho} \quad 0 \quad 0 \quad \frac{1}{\alpha P} \quad .$$

For $\alpha = \gamma$ this is the isentropic wall and for $\alpha = 1$ this is the isothermal or constant temperature wall.

The second row of T^{-1} , for the tangential velocity equation, involves the direction cosines for the local tangent to the η constant coordinate lines. Thus at the wall the condition that blown flux enter the flow normal to the wall can be expressed as the inner product (the tangential velocity component) $\hat{n}_y' u - \hat{n}_x' v = 0$. When differentiated this relation yields the same matrix representation for T' as the second row of T^{-1} . The third row of T^{-1} , for the P^+ pressure normal velocity compatibility equation, contains in columns two and three the direction cosines \hat{n}_x' and \hat{n}_y' for the local normals to the η constant coordinate lines. Many ablators of current and potential use sublimate at a nearly constant temperature, and the mass flow rate is proportional to the heating rate with a coefficient weakly dependent on the pressure. For convenience the pressure dependence can be described locally logarithmically. Then the auxiliary boundary condition for the mass flux can be written as a variation about a local reference heating state as

$$\frac{1}{\dot{m}} \delta \dot{m} - \frac{1}{\beta P} \delta P = \frac{1}{\dot{Q}} \delta \dot{Q} \quad (17)$$

Here $\dot{m} = \hat{n}_x' \rho u + \hat{n}_y' \rho v = \rho W^\eta$ and the left hand side takes the T' matrix representation

$$0 \quad \frac{\hat{n}_x'}{\rho W^\eta} \quad \frac{\hat{n}_y'}{\rho W^\eta} \quad - \frac{1}{\beta P}$$

Row one of T' is written for the primitive variable differences $\delta\rho$ and δP , while rows two and three are for the conservative variable differences $\delta(\rho u)$ and $\delta(\rho v)$. The fourth row of T' is immaterial since it is not selected by the D^+ truth function and in fact need not be programmed at all. The M' that constructs the above desired combination of primitive and conservative variable differences from the homogeneous conservative variable difference vector can be chosen as

$$\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \frac{u^2 + v^2}{2} & -u & -v & 1 \end{array}$$

IV. Results

An indication of the potential effectiveness of the CSCM method can be found in the results of two model problems.

The first model problem is the scalar Burgers equation ramp wave with inflow boundary condition and computed outflow. Here the single eigenvalue corresponding to \tilde{A} of a system is simply \bar{u} and the equation solved is

$$\delta u_i + \bar{u}_{i-\frac{1}{2}} \nabla_i u = 0 \quad \text{for } \bar{u} > 0. \quad (18)$$

In Figure 1a. the computed solution (boxes) is shown at three times (0.67, 1.33, 2.0) on the interval $.5 \leq x < 1$ for initial conditions $u = x$ on the interval. The exact solution $u = \frac{x}{1+t}$ plotted in

triangles connected by solid line has been given by Yee, Beam, and Warming²⁷ with computations that can be compared Figure 1b. The solution obtained with the present method was run explicitly at a Courant number of 0.8 and can be seen to be effectively exact. In particular there is no evidence of disconnectedness on the expansion indicating the method possesses a desirable degree of natural numerical dissipation.

The second model problem is Shubins hyperbolic tangent nozzle problem with supersonic inflow and subsonic outflow. The author is indebted to Warming and Yee for assistance in this problem by providing Shubins data and a code in which the method for the quasi 1-D Euler equations could conveniently be incorporated. Solution (Figures 2b. and 2c.), for this problem with different methods have been published by Yee²⁵ and by Yee, Beam, and Warming²⁷. In Figure 2a. a solution is shown at 1000 steps from an explicit calculation made with the present method at a Courant number of 0.8. For practical purposes the solution was obtained in 400-500 steps. The results, shown in boxes, can be seen to correspond to Shubins effectively exact solution to within the resolution of his data, shown connected by solid line. Again no difficulty is found with the expansion but also no noticeable smoothing of the jump transition is apparent.

A comment on accuracy, the graphs have been labeled "first order upwind" after the finite difference convention of simple one sided differences employed for these results. However, owing to the fact that the method's eigenvalues are effectively centered (the averaging procedure), the CSCM method is second order from a method of characteristics

point of view, Rakich^{*}. In any case, within the remarkable framework of Roe, the present finite difference method is extendable to any order of finite difference accuracy based on Taylor series.

V. Summary

A new conservative quasi one dimensional flux difference splitting has been presented for the hyperbolic terms of multidimensional gas-dynamics. The splitting based on local linearizing combinations of non-conservative primitive difference equations for one curvilinear coordinate direction is akin to a 1-D unsteady method of characteristics. In this respect the method is philosophically in accord with the split coefficient matrix method of Chakravarthy. But, unlike Chakravarthy and in accord with Roe, emphasis is placed on developing a method that maintains the global conservation property available in methods based on simple one sided conservative flux differences. To this end and extending the theoretical foundations of Roe's method, an elemental simple interval difference equation is defined out of which any globally conservative finite difference method can be constructed. Akin to how the conservative PDE's are constructed from the nonconservative primitive equations, a matrix transform of a discrete set of primitive difference equations is constructed to realize identically the conservative elemental interval equations. For application to real gas as well as perfect gas flows, the volumetric internal energy is chosen as the basis of the primitive equations representation rather than the pressure.

^{*}private conversation

Neither the primitive difference equations nor their transform, the characteristic equations, are solved but are only constructed conceptually in the matrix splitting of the conservative elemental interval equations. The split pieces of the latter, for which the characteristic equations may be regarded as eigenfunctions, are the basis of the nodal point finite difference equations that are solved in the conservative variables. Following the approach of Roe, stable nodal point difference equations are constructed by choosing split elemental interval equation pieces that provide upwind differencings according to the eigenvalues of the associated characteristic equations.

For application to direct implicit matrix methods it is necessary, in the delta form, to at least express the time difference of the spatial difference of the fluxes in terms of the spatial difference of the time differences of the conservative variables. In flux splitting as the result of the homogeneous property the flux can be expressed as the product of the Jacobian matrix and the conservative variable vector. The delta form follows. In the present work a further matrix transform has been found that exactly expresses the elemental interval primitive difference equations in terms of differences of the conservative variables. Thus with the conservative transform of the primitive equations, it has been possible in the present method to express the flux difference as a matrix transform of the primitive variable differences, hence the nomenclature flux difference splitting and the delta form also follows.

Finally the split elemental interval equation pieces corresponding to stable upwind characteristic equations to the boundaries are used in conjunction with auxiliary boundary conditions according to the

approach of Kentzer to form stable boundary point difference relations that are wholly consistent with the interior point conservative formulation.

Results of two model problems for which computations have previously been reported in the literature have been presented. The solution for the first problem, the Burgers equation ramp expansion, found effectively the exact solution with no evidence of oscillation or disconnectedness (expansion shocks) developing. The solution for the second model problem, Shubin's nozzle with supersonic inflow and subsonic outflow has also been found to be effectively exact including the shock location.

VI. Conclusions

A stable conservative finite difference method has been constructed that supports approximately the correct wave propagation and domain of dependence of characteristic methods. The splitting is sufficiently general to lend itself to a variety of numerical schemes, explicit or implicit, iterative or direct, for marching in time or space for the compressible Euler and Navier-Stokes equations. Based on preliminary results of model problems the upwind split method has the potential for both improved robustness and accuracy relative to the present generation of unsplit methods.

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Appendix A

Supra-Characteristic Matrices

We couch the discussion in terms of the 2-D axisymmetric 3-D flow equations which embody as elements the essential mathematical richness of all other cases of interest, i.e. 1-D, quasi 1-D, 2-D and 3-D. For a fixed computational mesh based on general curvilinear coordinates, the discrete finite volume difference analog of the maximally, conservative partial differential equation can be written

$$\begin{aligned}
 \hat{J} \delta_t \rho + \delta_\xi (\rho \hat{W}^\xi) + \delta_\eta (\rho \hat{W}^\eta) &= 0 \\
 \hat{J} \delta_t \rho u + \delta_\xi (\rho u \hat{W}^\xi + \hat{\xi}_x p) + \delta_\eta (\rho u \hat{W}^\eta + \hat{\eta}_x p) &= 0 \\
 \hat{J} \delta_t \rho v + \delta_\xi (\rho v \hat{W}^\xi) + \hat{\xi}_y \delta_\xi p + \delta_\eta (\rho v \hat{W}^\eta) + \hat{\eta}_y \delta_\eta p &= 0 \\
 \hat{J} \delta_t E + \delta_\xi ((E + p) \hat{W}^\xi) + \delta_\eta ((E + p) \hat{W}^\eta) &= 0
 \end{aligned} \tag{A1}$$

where $E = \frac{p}{\gamma-1} + \frac{1}{2} \rho (u^2 + v^2)$.

In the equations $\hat{W}^\xi = \hat{\xi}_x u + \hat{\xi}_y v$, and $\hat{W}^\eta = \hat{\eta}_x u + \hat{\eta}_y v$, are the cell face area weighted, contravariant velocity components, and the metric quantities $\hat{\xi}_x = \delta_\eta \frac{y^2}{2}$, $\hat{\xi}_y = -y \delta_\eta x$, $\hat{\eta}_x = -\delta_\xi \frac{y^2}{2}$, $\hat{\eta}_y = y \delta_\xi x$ are the x and y projections of the mesh cell face areas, and $\hat{J} = \delta_\xi \frac{y}{2} \hat{\xi}_y + \delta_\eta \frac{y}{2} \hat{\eta}_y$ is the volume of the associated computational cell. We note here the v momentum equation does not admit a strong

conservation law for the pressure; and we see no reason to introduce a weak one with the associated source term that may compromise numerical stability.

It is interesting that the quasi 1-D stream tube equations also have the same property of failing to admit a strong conservation law for the pressure term of the momentum equation. Indeed a valid representation of the latter set of equations can be obtained from the set A1 by dropping the η coordinate differenced terms and the u terms including the entire u momentum equation, then replacing v by u and ξ_y by ξ_x in the remainder. Of course the pure 1-D, 2-D, and 3-D flow formulations admit strong conservation laws like the u momentum equation of A1, for all the momentum equations of their respective sets.

The gasdynamic equations A1 are valid for equilibrium and nonequilibrium real gases as well as perfect gases so long as the times for relaxing internal atomic and molecular degrees of freedom are short compared with local residence and reaction times and a local thermodynamic equilibrium may be considered to exist. Such real gases (Reference 28) are subject to a gas law

$$p = \rho R T \quad (A2)$$

derived for a mixture of ideal gases of the real gas composition, and the appropriate γ for such a system is the specific enthalpy to internal energy ratio $\frac{h}{e}$. In order to preserve the real gas capability of the conservative gasdynamic equations A1 in the supra-characteristic splittings of derived primitive equations, it is most natural to express

A1 and the derived equations in the primitive variable $P \equiv \frac{p}{\gamma-1}$ rather than the pressure p .

Now with the realization fostered in the body of the report that we can maintain global conservation while treating each curvilinear coordinate direction autonomously, we will restrict the remainder of the discussion to splitting the flux difference terms for the η coordinate direction. Then the corresponding relations for the ξ coordinate direction can be obtained trivially by replacing the η super or subscripts by the appropriate ξ assuming the associated metric relations.

With the introduction of the primitive variable P defined above, it can be verified by straightforward algebraic manipulation that under the matrix multiplication M a vector of primitive equation elemental interval differences $\Delta_{\eta} \tilde{f}$ can be found to identically satisfy the elemental interval flux differences of the conservative equation $\Delta_{\eta} F$. The transforming matrix M in question is

$$\begin{array}{cccc}
 1 & 0 & 0 & 0 \\
 \bar{u} & 1 & 0 & 0 \\
 \bar{v} & 0 & 1 & 0 \\
 \frac{\bar{u}^2 + \bar{v}^2}{2} & \bar{u} & \bar{v} & 1
 \end{array} \quad (A3)$$

The right multiplying vector of primitive equation elemental interval differences $\Delta_{\eta} \tilde{f}$ is

$$\begin{aligned}
& \overline{\rho} \Delta_{\eta} \hat{W}^{\eta} + \overline{\hat{W}^{\eta}} \Delta_{\eta} \rho \\
& \overline{\rho \hat{W}^{\eta}} \Delta_{\eta} u + \Delta_{\eta} (\hat{\eta}_x (\gamma-1)P) \\
& \overline{\rho \hat{W}^{\eta}} \Delta_{\eta} v + \frac{\overline{\hat{\eta}_y v}}{\bar{v}} \Delta_{\eta} ((\gamma-1)P) \\
& \overline{\gamma P \hat{\eta}_x} \Delta_{\eta} u + \overline{\gamma P} \Delta_{\eta} \hat{\eta}_y v + \overline{u} \Delta_{\eta} (\hat{\eta}_x P) + \overline{v \hat{\eta}_y} \Delta_{\eta} P
\end{aligned} \tag{A4}$$

and the corresponding vector of elemental interval maximally conservative flux differences $\Delta_{\eta} F$ is

$$\begin{aligned}
& \Delta_{\eta} \rho \hat{W}^{\eta} \\
& \Delta_{\eta} \rho u \hat{W}^{\eta} + \Delta_{\eta} (\hat{\eta}_x (\gamma-1)P) \\
& \Delta_{\eta} \rho v \hat{W}^{\eta} + \frac{\overline{\hat{\eta}_y v}}{\bar{v}} \Delta_{\eta} ((\gamma-1)P) \\
& \Delta_{\eta} (\gamma P \hat{W}^{\eta} + \frac{1}{2}(u^2 + v^2)_{\rho} \hat{W}^{\eta}) .
\end{aligned} \tag{A5}$$

In the relation and as described in the body of the report, the bar over quantities represents the simple average of the values of the quantities at either end of the elemental difference interval, $(K, K+1)$ for η .

The primitive variable time differences associated with A4 are given by the (column) vector $J (\delta_t \rho, \rho \delta_t u, \rho \delta_t v, \delta_t P)^*$ (A6). These multiplied by A3 can be seen to provide measures of the conservative variable time differences.

Elemental difference supra-characteristic equations can be formed of A4 and A6 by multiplying by the matrix T^{-1} which is

$$\begin{array}{cccc}
 -\frac{1}{\bar{\rho}} & 0 & 0 & \frac{1}{\bar{\gamma}P} \\
 0 & \frac{\bar{\hat{n}}'_y}{\bar{\rho}\bar{c}} & -\frac{\bar{\hat{n}}'_x}{\bar{\rho}\bar{c}} & 0 \\
 0 & \frac{\bar{\hat{n}}'_x}{\bar{\rho}\bar{c}} & \frac{\bar{\hat{n}}'_y}{\bar{\rho}\bar{c}} & \frac{1}{\bar{\gamma}P} \\
 0 & \frac{-\bar{\hat{n}}'_x}{\bar{\rho}\bar{c}} & \frac{-\bar{\hat{n}}'_y}{\bar{\rho}\bar{c}} & \frac{1}{\bar{\gamma}P}
 \end{array} \quad (A7)$$

Here the primed averaged metric quantities are the averaged quantities divided by the square root of the sum of their squares or the averaged cell face area. In fact, see section III, the primed quantities as used in columns 2 and 3 above provide respectively the x and y direction cosines of the tangent (row 2) and normal (rows 3 and 4) to the local mean η constant coordinate surface. Based on the natural normalizations of the primitive equations, the transformation A7 linearizes the quasi 1-D elemental difference equations into near orthogonal combinations of variables that approximate with first order truncation error scalar difference equations. It is well to emphasize here that the intent is not to solve such equations in characteristic variables but only to use the resulting near orthogonality as an intermediate step to obtain a well conditioned matrix formulation in the conservative variables. By row, the intermediate equations resulting from A7 support the quasi one dimensional propagation of local variations in entropy, tangential velocity, and the P^+ and P^- pressure-normal velocity compatibility relations.

The eigenvalues associated with the approximately scalar transformed equations are by row \hat{W}^n , \hat{W}^n , $\hat{W}^n + \hat{n}_c$, $\hat{W}^n - \hat{n}_c$. In the method (section II) these eigenvalues remain embedded in the spatial difference terms of the primitive equations which are treated exactly. Only the sign of the eigenvalues is tested to determine where (forward or backward) split pieces of such terms should be "sent", in the sense of Roe, to form stable nodal difference equations.

The inverse T of the matrix T^{-1} is

$$\begin{array}{cccc}
 -\bar{\rho} & 0 & \frac{\bar{\rho}}{2} & \frac{\bar{\rho}}{2} \\
 0 & \bar{\rho}\bar{c}\hat{n}_y' & \frac{\bar{\rho}\bar{c}}{2}\hat{n}_x' & -\frac{\bar{\rho}\bar{c}}{2}\hat{n}_x' \\
 0 & -\bar{\rho}\bar{c}\hat{n}_x' & \frac{\bar{\rho}\bar{c}}{2}\hat{n}_y' & -\frac{\bar{\rho}\bar{c}}{2}\hat{n}_y' \\
 0 & 0 & \frac{\bar{\gamma}P}{2} & \frac{\bar{\gamma}P}{2}
 \end{array} \quad (A8)$$

the primitive variable spatial difference terms be expressed in terms of spatial differences of the conservative variables. This end is accomplished exactly by the matrix transform $\tilde{M}(\Delta_\eta)q \equiv \Delta_\eta \tilde{f}$ with $\tilde{M}(\Delta_\eta)$ given in Table A1. Then with the identity $\Delta_\eta F = M\Delta_\eta \tilde{f}$, the splittable linearizing formulation sketched in relations (1) and (8) of the body of the report follows by

$$\Delta_\eta F = M \tilde{M}^{-1}(\Delta_\eta)q = M T D T^{-1} \tilde{M}^{-1}(\Delta_\eta)q \quad (A9)$$

where recall $D = D^+ + D^- = I$, the identity matrix.

Table A1. Conservative variable transform for elemental primitive equation spatial difference terms

0	$\Delta_n \hat{n}_x$	$\Delta_n \hat{n}_y$	0
$-\frac{\overline{\rho \hat{W} \eta \bar{u}}}{\bar{\rho}} \Delta_n - \frac{\bar{S}^2}{2} \Delta_n \hat{n}_x (\gamma-1)$	$\frac{\overline{\rho \hat{W} \eta}}{\bar{\rho}} \Delta_n$	$-\frac{(\gamma-1) \overline{\rho \hat{n}_x}}{\bar{\rho}} \bar{v} \Delta_n$	$\Delta_n \hat{n}_x (\gamma-1)$
$\frac{(\gamma-1) \overline{\rho \hat{n}_x}}{\bar{\rho}} \bar{S}^2 \Delta_n$	$-\frac{(\gamma-1) \overline{\rho \hat{n}_x \bar{u}}}{\bar{\rho}} \Delta_n$		
$-\frac{\overline{\rho \hat{W} \eta \bar{v}}}{\bar{\rho}} \Delta_n - \frac{\bar{S}^2}{2} \frac{\hat{n}_y \bar{v}}{\bar{v}} \Delta_n (\gamma-1)$	$-\frac{(\gamma-1) \overline{\rho \hat{n}_y \bar{v}}}{\bar{\rho}} \bar{u} \Delta_n$	$\frac{\overline{\rho \hat{W} \eta}}{\bar{\rho}} \Delta_n$	$\frac{\hat{n}_y \bar{v}}{\bar{v}} \Delta_n (\gamma-1)$
$\frac{(\gamma-1) \overline{\rho \hat{n}_y \bar{v}}}{\bar{\rho}} \bar{S}^2 \Delta_n$		$-\frac{(\gamma-1) \overline{\rho \hat{n}_y \bar{v}}}{\bar{\rho}} \bar{v} \Delta_n$	
$-\frac{\gamma \bar{P} \overline{\hat{n}_x}}{\bar{\rho}} \bar{u} \Delta_n - \frac{\gamma \bar{P}}{\bar{\rho}} \overline{\hat{n}_y \bar{v}} \Delta_n$	$\frac{\gamma \bar{P} \overline{\hat{n}_x}}{\bar{\rho}} \Delta_n$	$\frac{\gamma \bar{P}}{\bar{\rho}} \Delta_n \hat{n}_y$	$\bar{u} \Delta_n \hat{n}_x$
$\overline{\hat{n}_y \bar{v}} (\bar{S}^2 - \frac{\bar{S}^2}{2}) \Delta_n$	$-\overline{\hat{n}_y \bar{v}} \bar{u} \Delta_n$	$-\overline{\hat{n}_y \bar{v}} \bar{v} \Delta_n$	$\overline{\hat{n}_y \bar{v}} \Delta_n$
$\frac{\overline{\hat{n}_x \rho}}{\bar{\rho}} \bar{u} \bar{S}^2 \Delta_n - \bar{u} \frac{\bar{S}^2}{2} \Delta_n \hat{n}_x$	$-\frac{\overline{\hat{n}_x \rho}}{\bar{\rho}} \bar{u}^2 \Delta_n$	$-\frac{\overline{\hat{n}_x \rho}}{\bar{\rho}} \bar{u} \bar{v} \Delta_n$	

Note $\bar{S}^2 = \bar{u}^2 + \bar{v}^2$ and $\bar{S}^2 = \bar{u}^2 + \bar{v}^2$

Finally the specification of $\tilde{\tilde{A}}$, defined in the body of the report for the unsteady terms (see equations (10) and (11)) by

$$\tilde{\tilde{A}} = M T D T^{-1} M^{-1}, \quad (A10)$$

is completed here with the matrix inverse of M . The inverse M^{-1} is

$$\begin{array}{cccc} 1 & 0 & 0 & 0 \\ -\bar{u} & 1 & 0 & 0 \\ -\bar{v} & 0 & 1 & 0 \\ \bar{u}^2 + \bar{v}^2 & -\bar{u} & -\bar{v} & 1 \\ -\frac{1}{2}(\bar{u}^2 + \bar{v}^2) & & & \end{array}$$

CSCM First Order Upwind

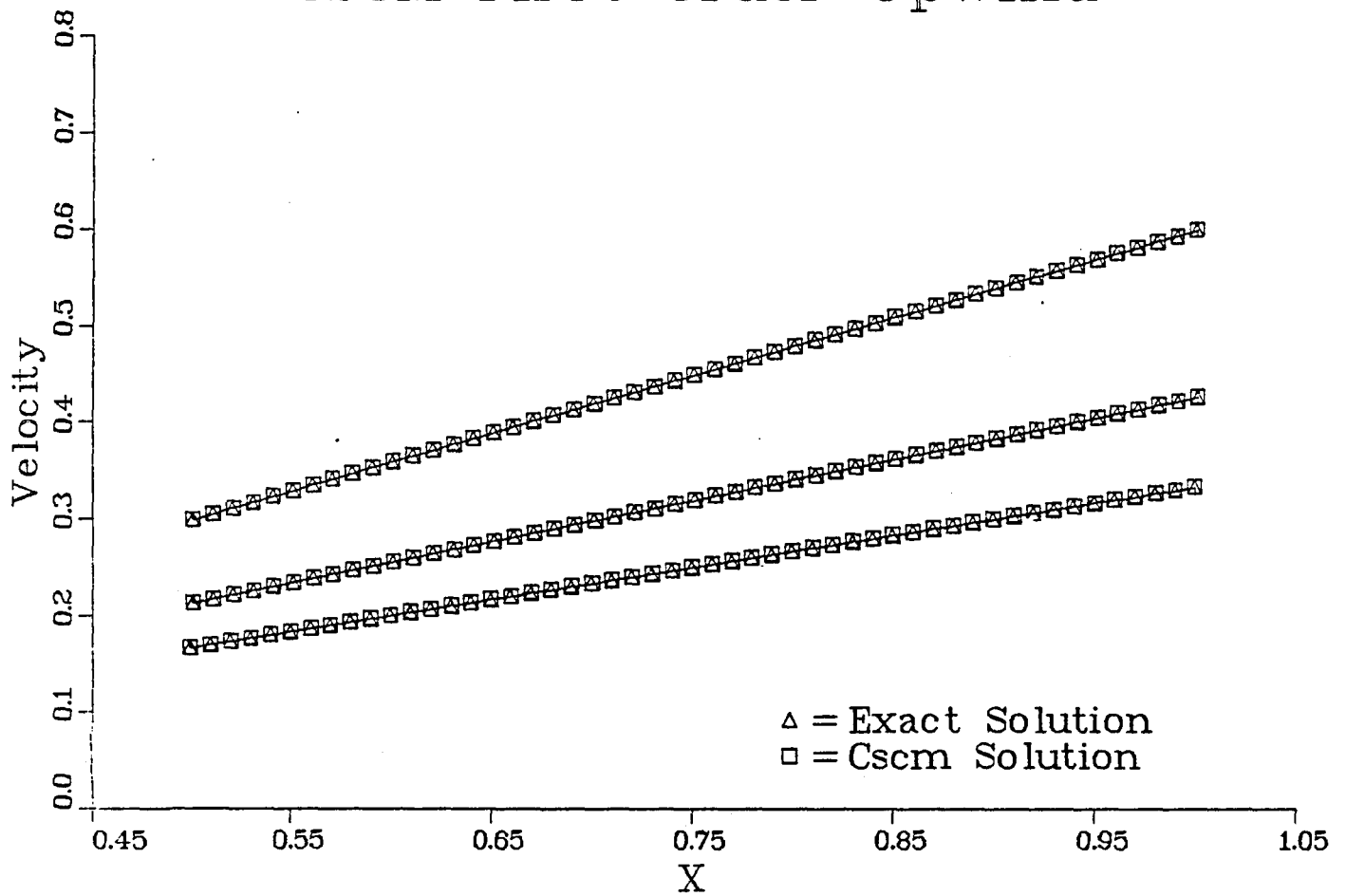


Figure 1a. Burgers equation solution shown in boxes for the ramp expansion by present CSCM method. Exact solution in triangles connected by solid line.

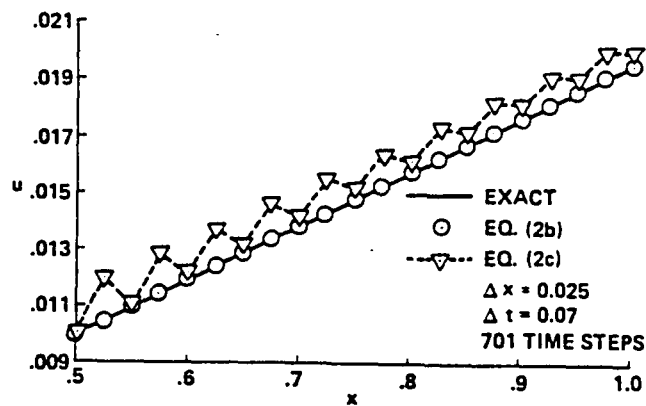


Figure 1b. Burgers equation solution for the ramp expansion, reference 27.

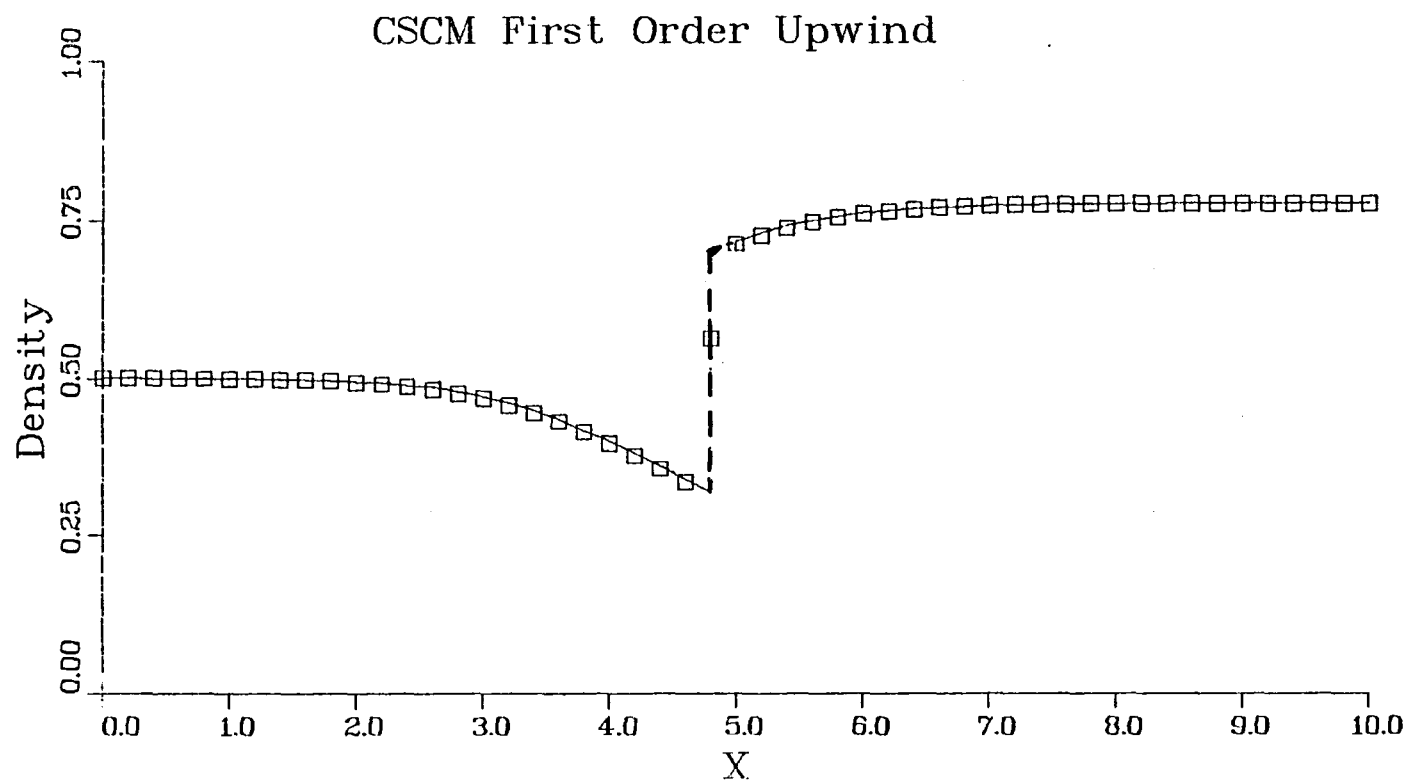


Figure 2a. Shubins nozzle solution shown in boxes, supersonic inflow, subsonic outflow by present CSCM method. Exact solution points connected by solid line.

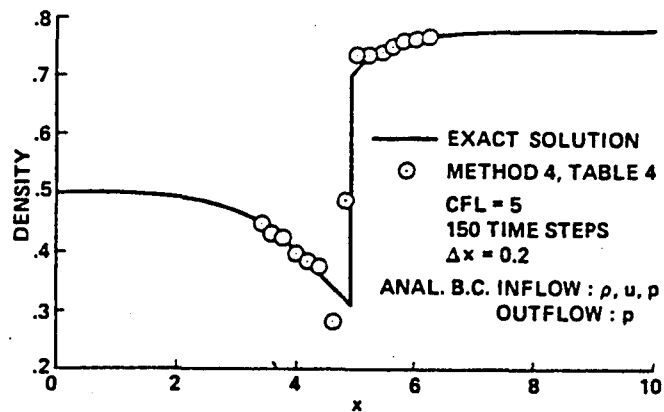


Figure 2b. Shubins nozzle, supersonic inflow, subsonic outflow, solution as shown in reference 27.

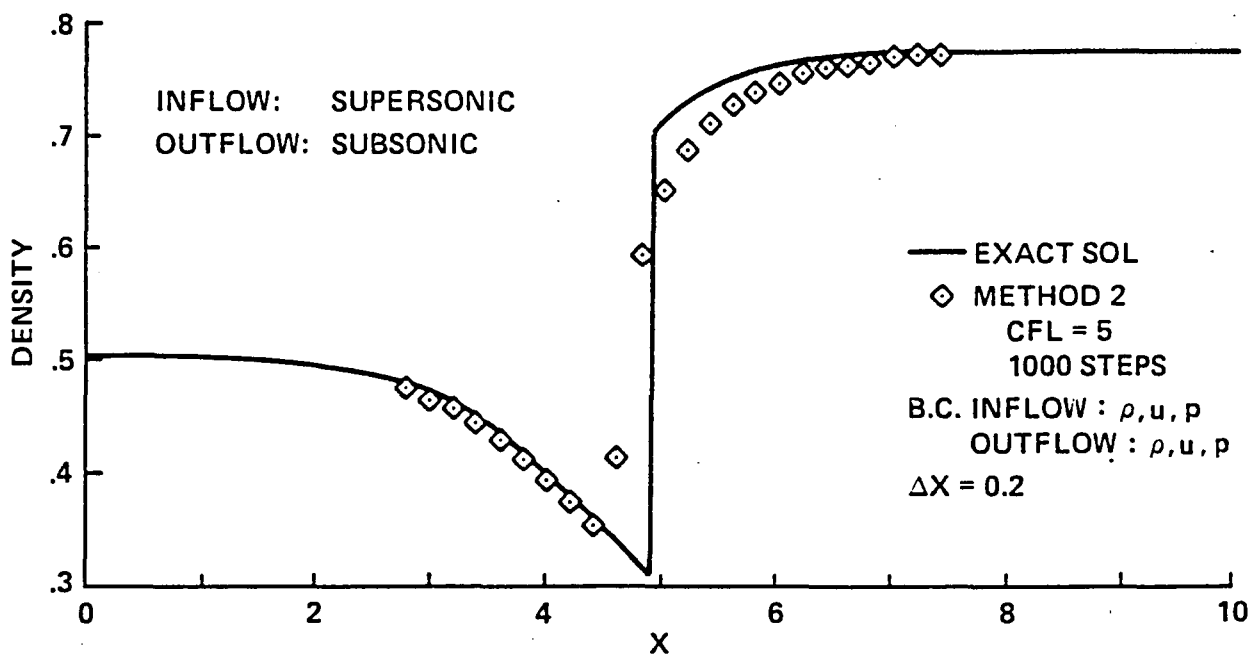


Figure 2c. Shubins nozzle, supersonic inflow, subsonic outflow, solution as shown in reference 25.

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16. Abstract A new conservative flux difference splitting is presented for the hyperbolic systems of gasdynamics. The stable robust method is suitable for wide application in a variety of schemes, explicit or implicit, iterative or direct, for marching in either time or space. The splitting is modeled on the local quasi one dimensional characteristics system for multi-dimensional flow similar to Chakravarthy's nonconservative split coefficient matrix method (SCM); but, as the result of maintaining global conservation, the method is able to capture sharp shocks correctly. The embedded characteristics formulation is cast in a primitive variable the volumetric internal energy (rather than the pressure) that is effective for treating real as well as perfect gases. Finally the relationship of the splitting to characteristics boundary conditions is discussed and the associated conservative matrix formulation for a computed blown wall boundary condition is developed as an example. The theoretical development employs and extends the notion of Roe of constructing stable upwind difference formulae by "sending" split simple one sided flux difference pieces to appropriate mesh sites. The developments are also believed to have the potential for aiding in the analysis of both existing and new conservative difference schemes.			
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